

**WHAT IS CLAIMED IS:**

1. A method of selecting sample tube-solvent pairs for performing nuclear magnetic resonance measurements, comprising:
  - a) determining a first frequency shift introduced by a first sample into a resonant circuit of a nuclear magnetic resonance spectrometer, the first sample including a first sample tube containing a first sample solvent and a first compound of interest, wherein the first solvent has a first solvent dielectric constant and the first sample tube has a first effective sample tube dielectric constant;
  - b) determining a second frequency shift introduced by a second sample into a resonant circuit of a nuclear magnetic resonance spectrometer, the first sample including a first sample tube containing a first sample solvent and a first compound of interest, wherein the second solvent has a second solvent dielectric constant different from the first solvent dielectric constant, and the second sample tube has a second effective sample tube dielectric constant different from the first sample tube dielectric constant;
  - c) determining whether a relationship between the first frequency shift and the second frequency shift meets a predetermined condition; and
  - d) selecting the first sample and the second sample for performing nuclear magnetic resonance measurements on the first compound of interest and the second compound of interest if the relationship between the first frequency shift and the second frequency shift meets the predetermined condition.
2. The method of claim 1, wherein determining whether the relationship between the first frequency shift and the second frequency shift meets the predetermined condition comprises determining whether a difference between the first frequency shift and the second frequency shift is less than or equal to a predetermined value.
3. The method of claim 2, wherein the predetermined value is less than or equal to a -5 dB bandwidth of a nuclear magnetic resonance probe to be used for the measurements.

4. The method of claim 2, wherein the predetermined value is less than or equal to a -  
10 dB bandwidth of a nuclear magnetic resonance probe to be used for the  
measurements.
- 5 5. The method of claim 2, wherein the predetermined value is less than or equal to  
0.8 MHz.
6. The method of claim 2, wherein the predetermined value is less than or equal to  
0.4 MHz.
- 10 7. The method of claim 6, wherein a magnitude of a difference between the first solvent  
dielectric constant and the second solvent dielectric constant is higher than ten.
8. The method of claim 2, wherein the predetermined value is less than or equal to  
0.2 MHz.
- 15 9. The method of claim 1, wherein the first sample tube dielectric constant is higher than  
or equal to 20.
- 20 10. The method of claim 9, wherein the second sample tube dielectric constant is lower  
than or equal to 10.
11. The method of claim 10, wherein the first solvent is apolar, and the second solvent is  
polar.
- 25 12. The method of claim 9, wherein the second sample tube is formed from a material  
selected from quartz, sapphire, borosilicate glass, and plastic.
13. The method of claim 1, wherein the first sample tube dielectric constant is higher than  
or equal to 100.
- 30 14. The method of claim 1, wherein the first sample tube comprises a ceramic.
15. The method of claim 1, wherein the first sample tube is formed by a monolithic piece.

16. The method of claim 1, wherein the first sample tube comprises two layers of materials having different dielectric constants.
- 5 17. The method of claim 16, wherein one of the two layers is a coating disposed on another of the two layers.
18. The method of claim 1, wherein the first sample tube comprises an outer shell and a rod positioned within the outer shell.
- 10 19. The method of claim 1, further comprising sequentially performing nuclear magnetic resonance measurements on the first sample and the second sample using the resonant circuit.
- 15 20. The method of claim 19, wherein between a measurement performed on the first sample and a measurement performed on the second sample, the resonant circuit is not externally retuned to compensate for the difference between the first frequency shift and the second frequency shift.
- 20 21. The method of claim 19, wherein the first frequency shift and the second frequency shift are substantially equal.
22. The method of claim 1, wherein determining the first frequency shift and the second frequency shift comprises looking up pre-measured values of the first frequency shift and the second frequency shift.
- 25 23. A method of selecting sample tubes for performing tuning-compensated nuclear magnetic resonance measurements, comprising:
- 30 a) determining a first frequency shift introduced in a resonant frequency of a resonant circuit of a nuclear magnetic resonant spectrometer by a first sample comprising a first sample tube containing a first sample solvent;
- b) determining a second frequency shift introduced in the resonant frequency of the resonant circuit by a second sample comprising a second sample tube containing a second sample solvent, wherein the first sample solvent is

- different from the second sample solvent and the first sample tube has a different effective dielectric constant from the second sample tube; and
- c) if the first frequency shift is substantially equal to the second frequency shift, selecting the first sample and the second sample for sequentially performing nuclear magnetic resonance measurements using the resonant circuit on a first compound of interest contained in the first solvent in the first sample tube and on a second compound of interest contained in the second solvent in the second sample tube.

24. The method of claim 23, further comprising a step of selecting the second sample tube such that

$$A\ln(\epsilon_{st1}+1) + B\ln(\epsilon_{s1}+1) = A\ln(\epsilon_{st2}+1) + B\ln(\epsilon_{s2}+1),$$

wherein A and B are numeric constants,  $\epsilon_{st1}$  is a dielectric constant of the first sample tube,  $\epsilon_{st2}$  is a dielectric constant of the second sample tube,  $\epsilon_{s1}$  is a dielectric constant of the first solvent, and  $\epsilon_{s2}$  is a dielectric constant of the second solvent.

25. A method of performing tuning-compensated nuclear magnetic resonance measurements, comprising:

- a) loading a first sample into a nuclear magnetic resonance probe of a nuclear magnetic resonance spectrometer, the first sample including a first sample tube containing a first sample solvent and a first compound of interest, the spectrometer including a resonant circuit for performing nuclear magnetic resonance measurements on samples, wherein the first solvent has a first solvent dielectric constant and the first sample tube has a first sample tube dielectric constant, and the first sample causes a first frequency shift in the resonant frequency of the resonant circuit upon loading into the probe;
- b) employing the resonant circuit to perform a first nuclear magnetic resonance measurement on the first compound of interest contained in the first sample tube;
- c) after the first nuclear magnetic resonance measurement is performed, loading a second sample including a second sample tube containing a second sample

solvent and a second compound of interest into the nuclear magnetic resonance probe, wherein

the second solvent has a second solvent dielectric constant different from the first solvent dielectric constant,

the second sample tube has a second sample tube dielectric constant different from the first sample tube dielectric constant,

the second sample causes a second frequency shift in the resonant frequency of the resonant circuit upon loading into the probe; and

d) employing the resonant circuit to perform a second nuclear magnetic resonance measurement on the compound of interest contained in the second sample tube;

wherein the second frequency shift is substantially equal to the first frequency shift, whereby the resonant frequency of the resonant circuit need not be externally retuned between the first nuclear magnetic resonance measurement and the second nuclear magnetic resonance measurement.

26. The method of claim 25, wherein the first sample tube dielectric constant is higher than or equal to 20.

27. The method of claim 26, wherein the second sample tube dielectric constant is lower than or equal to 10.

28. The method of claim 27, wherein the first solvent is apolar, and the second solvent is polar.

29. The method of claim 26, wherein the second sample tube is formed from a material selected from quartz, sapphire, borosilicate glass, and plastic.

30. The method of claim 25, wherein the first sample tube dielectric constant is higher than or equal to 100.

31. The method of claim 25, wherein the first sample tube comprises a ceramic.

32. The method of claim 25, wherein a magnitude of a difference between the first solvent dielectric constant and the second solvent dielectric constant is higher than or equal to 10, and a magnitude of a difference between the first sample tube dielectric constant and the second sample tube dielectric constant is higher than or equal to 10.

5

33. The method of claim 25, wherein the first solvent is water.

34. The method of claim 33, wherein the second solvent is selected from benzene and chloroform.

10

35. The method of claim 25, wherein the first sample tube is formed by a monolithic piece.

36. The method of claim 25, wherein the first sample tube comprises two layers of materials having different dielectric constants.

15

37. The method of claim 25, wherein the first sample tube comprises an outer shell and a rod positioned within the outer shell.

20

38. The method of claim 25, further comprising:

- a) loading a batch of samples into a sample holder, the batch of samples including the first sample and the second sample; and
- b) sequentially transferring the batch of samples from the sample holder to the probe.

25

39. A method of performing tuning-compensated nuclear magnetic resonance measurements, comprising:

- a) performing a first nuclear magnetic resonance measurement on a first sample, the first sample comprising a first sample tube containing first sample contents including a first sample solvent and a first compound of interest;
- b) performing a second nuclear magnetic resonance measurement on a second sample, the second sample comprising a second sample tube containing second sample contents including a second sample solvent and a second compound of interest; wherein

30

an effective dielectric constant of the first sample tube is lower than an effective dielectric constant of the second sample tube, a dielectric constant of the first sample contents is higher than a dielectric constant of the second sample contents, whereby a difference in dielectric properties between the first sample tube and the second tube compensates at least partially for a difference in dielectric properties between the first sample contents and the second sample contents.

40. The method of claim 41, wherein the effective dielectric constant of the second sample tube is higher than or equal to 20.

41. A method of performing tuning-compensated nuclear magnetic resonance measurements, comprising:

- a) loading a first solvent and a first set of compounds of interest into a corresponding plurality of substantially identical first sample tubes, wherein each first sample tube containing the first solvent introduces a first frequency shift into a resonant frequency of a resonant circuit of a nuclear magnetic resonance spectrometer; and
- b) loading a second solvent and a second set of compounds of interest into a corresponding plurality of substantially identical second sample tubes different from the first sample tubes, the second solvent being different from the first solvent, wherein each second sample tube containing the second solvent introduces a second frequency shift into the resonant frequency of the resonant circuit, and wherein the second frequency shift is substantially equal to the first frequency shift;
- c) employing the resonant circuit to sequentially perform nuclear magnetic resonant measurements on the set of first compounds of interest loaded into the plurality of first sample tubes containing the first solvent, and on the set of second compounds of interest loaded into the plurality of second sample tubes containing the second solvent.

42. A method of performing tuning-compensated nuclear magnetic resonance measurements, comprising:

a) loading a first sample into a nuclear magnetic resonance probe of a nuclear magnetic resonance spectrometer, the first sample including a first sample tube containing a first sample solvent and a first compound of interest, the spectrometer including a resonant circuit for performing nuclear magnetic resonance measurements on samples, wherein the first solvent has a first solvent dielectric constant and the first sample tube has a first sample tube dielectric constant, and the first sample causes a first frequency shift in the resonant frequency of the resonant circuit upon loading into the probe;

b) employing the resonant circuit to perform a first nuclear magnetic resonance measurement on the first compound of interest contained in the first sample tube;

c) after the first nuclear magnetic resonance measurement is performed, loading a second sample including a second sample tube containing a second sample solvent and a second compound of interest into the nuclear magnetic resonance probe, wherein

the second solvent has a second solvent dielectric constant different from the first solvent dielectric constant,

the second sample tube has a second sample tube dielectric constant different from the first sample tube dielectric constant,

the second sample causes a second frequency shift in the resonant frequency of the resonant circuit upon loading into the probe; and

d) employing the resonant circuit to perform a second nuclear magnetic resonance measurement on the compound of interest contained in the second sample tube;

wherein a magnitude of a difference between the second frequency shift and the first frequency shift is lower than a -5 dB bandwidth of the probe.

43. The method of claim 42, wherein the magnitude of the difference between the second frequency shift and the first frequency shift is lower than a -10 dB bandwidth of the probe.

44. The method of claim 42, wherein a magnitude of a difference between the first solvent dielectric constant and the second solvent dielectric constant is higher than ten.



45. A method of performing tuning-compensated nuclear magnetic resonance measurements, comprising:

- 5 a) loading a first sample comprising a first sample tube containing a first solvent and a first compound of interest into a nuclear magnetic resonance probe of a nuclear magnetic resonance spectrometer, wherein the first solvent has a first solvent dielectric constant and the first sample tube has a first sample tube dielectric constant;
- 10 b) employing the probe and spectrometer to perform a first nuclear magnetic resonance measurement on the first compound of interest contained in the first sample tube;
- 15 c) after the first nuclear magnetic resonance measurement is performed, loading a second sample comprising a second sample tube containing a second solvent and a second compound of interest into the nuclear magnetic resonance probe, wherein:  
the second solvent has a second solvent dielectric constant different from the first solvent dielectric constant,  
the second sample tube has a second sample tube dielectric constant different from the first sample tube dielectric constant, and  
20 a difference between the first sample tube dielectric constant and the second sample tube dielectric constant substantially offsets a difference between the first solvent dielectric constant and the second solvent dielectric constant; and
- 25 d) employing the probe and spectrometer to perform a second nuclear magnetic resonance measurement on the second compound of interest contained in the second sample tube.

46. A method of performing tuning-compensated nuclear magnetic resonance measurements, comprising the steps of:

- 30 a) loading a first sample comprising a first sample tube containing a first solvent and a first compound of interest into a nuclear magnetic resonance probe of a nuclear magnetic resonance spectrometer, wherein the first sample has a first effective dielectric constant;

- b) performing a first nuclear magnetic resonance measurement on the first sample;
- c) after the first nuclear magnetic resonance measurement is performed, loading a second sample comprising a second sample tube containing a second solvent and a second compound of interest into the nuclear magnetic resonance probe, wherein the second sample has a second effective dielectric constant, and wherein:
  - the first solvent has a different dielectric constant from the second solvent,
  - the first sample tube has a different dielectric constant from the second sample tube, and
  - the first effective dielectric constant is substantially equal to the second effective dielectric constant; and
- d) performing a second nuclear magnetic resonance measurement on the second sample.

47. An apparatus for performing tuning-compensated nuclear magnetic resonance measurements, comprising:

- a) a nuclear magnetic resonance spectrometer including a resonant circuit for sequentially performing nuclear magnetic resonance measurements on samples inserted in a measurement location of the spectrometer; and
- b) a sample holding and loading system for storing and loading into the measurement location a plurality of samples, the plurality of samples comprising
  - a plurality of first samples comprising a plurality of sample tubes containing a first solvent and a corresponding first set of compounds of interest, wherein each first sample introduces a first frequency shift into a resonant frequency of the resonant circuit, and
  - a plurality of second samples comprising a plurality of second sample tubes containing a second solvent and a corresponding second set of compounds of interest, wherein
    - each of the second sample tubes has a different dielectric constant from each of the first sample tubes,
    - the second solvent has a different dielectric constant from the first solvent,

each second sample introduces a second frequency shift into the  
resonant frequency of the resonant circuit, and  
the second frequency shift is substantially equal to the first frequency  
shift.

5

48. A sample holder for storing a plurality of samples for sequential loading into a nuclear  
magnetic resonance spectrometer, comprising:

- a) a sample holder for holding the plurality of samples;
- b) a plurality of first samples situated in the sample holder, comprising a plurality  
of sample tubes containing a first solvent and a corresponding first set of  
compounds of interest, wherein each first sample introduces a first frequency  
shift into a resonant frequency of the resonant circuit; and
- c) a plurality of second samples situated in the sample holder, comprising a  
plurality of second sample tubes containing a second solvent and a  
corresponding second set of compounds of interest, wherein  
each of the second sample tubes has a different dielectric constant from each  
of the first sample tubes,  
the second solvent has a different dielectric constant from the first solvent,  
each second sample introduces a second frequency shift into the resonant  
frequency of the resonant circuit, and  
the second frequency shift is substantially equal to the first frequency shift.

10

15

20